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Synthesis and crystal structure of 3-*N*-acetyl-5-(pyridin-3-yl)-2-(quinolin-2-yl)-1,3,4-oxadiazoline, C₁₈H₁₄N₄O₂

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.45 × 0.44 × 0.40 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.09 mm ⁻¹
Diffractometer, scan mode:	Oxford Diffraction Gemini, omega scans
$\theta_{\max}$, completeness:	25.0°, 96%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	3916, 2736, 0.029
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1688
$N(\text{param})_{\text{refined}}$:	218
Programs:	CrysAlis ^{PRO} [1], Olex2 [2], SHELX [3, 4]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.9068(2)	0.39481(18)	0.3208(2)	0.0422(5)
O2	0.7590(3)	0.0015(2)	0.5539(2)	0.0575(6)
N1	0.7505(3)	0.2260(2)	0.4974(2)	0.0416(6)
N2	0.7144(3)	0.3405(2)	0.5279(3)	0.0418(6)
N3	0.9516(3)	0.7840(2)	0.2686(3)	0.0514(7)
N4	0.6239(3)	0.3030(2)	0.2498(2)	0.0383(6)
C1	0.8080(3)	0.4322(3)	0.4232(3)	0.0344(7)
C2	0.8777(4)	0.2529(3)	0.3643(3)	0.0384(7)
H2	0.9937	0.1900	0.3780	0.046*
C3	0.9303(4)	0.6579(3)	0.2907(3)	0.0432(8)
H3	0.9938	0.6267	0.2253	0.052*
C4	0.8186(4)	0.5703(3)	0.4059(3)	0.0338(7)
C5	0.7217(4)	0.6185(3)	0.5040(3)	0.0384(7)
H5	0.6451	0.5642	0.5815	0.046*
C6	0.7420(4)	0.7481(3)	0.4833(3)	0.0418(7)
H6	0.6800	0.7822	0.5469	0.050*
C7	0.8572(4)	0.8263(3)	0.3656(3)	0.0470(8)
H7	0.8700	0.9131	0.3528	0.056*
C8	0.8000(4)	0.2477(3)	0.2575(3)	0.0358(7)
C9	0.9168(4)	0.1899(3)	0.1694(3)	0.0419(7)
H9	1.0372	0.1511	0.1804	0.050*
C10	0.8507(4)	0.1919(3)	0.0687(3)	0.0488(8)
H10	0.9255	0.1540	0.0108	0.059*
C11	0.6653(4)	0.2529(3)	0.0529(3)	0.0432(8)
C12	0.5560(4)	0.3057(3)	0.1471(3)	0.0382(7)
C13	0.3697(4)	0.3666(3)	0.1346(3)	0.0507(8)

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Abstract

C₁₈H₁₄N₄O₂, triclinic, $P\bar{1}$ (no. 2), $a = 7.6557(7)$ Å, $b = 11.0905(8)$ Å, $c = 11.3544(9)$ Å, $\alpha = 61.6430(10)^\circ$, $\beta = 73.600(2)^\circ$, $\gamma = 75.397(2)^\circ$, $V = 805.86(11)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0609$, $wR_{\text{ref}}(F^2) = 0.1633$, $T = 298$ K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

In a representative experiment 3-methylquinolin (1.0 mmol) reacted with SeO₂ (1.1 mmol) in dioxane (10 mL) at 80 °C to

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Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
H13	0.2964	0.3997	0.1967	0.061*
C14	0.2982(5)	0.3765(4)	0.0314(4)	0.0668(10)
H14	0.1771	0.4165	0.0238	0.080*
C15	0.4085(6)	0.3259(4)	−0.0633(4)	0.0757(11)
H15	0.3592	0.3341	−0.1332	0.091*
C16	0.5878(6)	0.2649(4)	−0.0537(4)	0.0655(10)
H16	0.6581	0.2315	−0.1164	0.079*
C17	0.7078(4)	0.0961(3)	0.5885(3)	0.0422(8)
C18	0.6002(5)	0.0792(3)	0.7292(3)	0.0604(9)
H18A	0.5387	−0.0010	0.7715	0.091*
H18B	0.5110	0.1598	0.7206	0.091*
H18C	0.6831	0.0682	0.7843	0.091*

afford the aldehyde, and then the mixture was reacted with nicotinohydrazide (1.0 mmol) in acetic anhydride (5 mL). The reaction mixture was refluxed and the title compound was purified by preparative thin-layer chromatography (PTLC) and recrystallised from dichloromethane. ¹H NMR (400 MHz, Chloroform-*d*) δ [ppm]: 9.14 (d, *J* = 2.8 Hz, 1H), 8.73 (dd, *J* = 4.9, 1.2 Hz, 1H), 8.24 (d, *J* = 8.4 Hz, 1H), 8.13–8.18 (m, 2H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.74 (t, *J* = 7.2 Hz, 1H), 7.54–7.60 (m, 2H), 7.36–7.40 (m, 1H), 7.26 (m, 1H), 2.42 (s, 3H).

Experimental details

Crystal structure determination of C₁₈H₁₄N₄O₂ by X-ray diffractions was carried on a Oxford Diffraction Gemini with the crystal kept at 298 K during data collection. The structure was solved with the Olex2 program [2] as an interface together with the SHELXT and SHELXL programs [3, 4]. Hydrogen atoms were treated using a riding model.

Comment

Recent studies show that introduction of active fragments into quinolin could increase biological activity [5]. Oxazoline is a group of heterocyclic compounds with nitrogen and oxygen atoms, which showed bioactivities such as anti-HIV [6] and antibacterial [7] activities. To further study the structure-activity relationship of quinolin, here we introduced oxazoline ring and prepared an quinolin-based derivative to find compounds with potential activity.

The asymmetric unit of the title structure consists of one crystallographically independent molecule (shown in the

figure). One 1,3,4-oxadiazolyl group, one 3-pyridinyl ring and one quinolinyl moiety form the title molecule. All bond lengths are in normal ranges and they are similar with the known compound [8]. The short C–N bond length of 1.303(3) Å (N2–C1) suggests a localized double bond, and the C–N bond lengths of 1.486(3) Å (N1–C2) suggests a localized single bond. The bond distance of C17–O2 is 1.227(3) Å, which is typical for a carbonyl group.

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